

No spin diffusion in the spin 1/2 XXZ chain at $T = \infty$: Numerical asymptotics

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Abstract

We analyze the recent numerical computations made by Fabricius, Löw and Stolze to show that the long time behavior of the zz correlation function of the spin 1/2 XXZ chain at $T = \infty$ is very well fit by the formula $t^{-d}[A + Be^{-\gamma(t-t_0)} \cos \Omega(t-t_0)]$ where d is substantially greater than 1/2. This confirms the conclusion that there is no spin diffusion in this model.

1. Introduction

The spin 1/2 XXZ chain of N site with periodic boundary conditions specified by the Hamiltonian

$$H = \frac{1}{2} \sum_{i=1}^N (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z) \quad (1.1)$$

where σ_i^j is the $y = x, y, z$ Pauli spin matrix at site i is well known to be an integrable system. As such it is to be expected that all the spin correlation functions should be analytically computable. In the past decade there has been much work done to fulfill this promise but much still remains to be done. In particular there has been no published work done on the time dependent autocorrelation function at infinite temperature

$$S(t; \Delta) = \langle \sigma_0^z(t) \sigma_0^z(0) \rangle = \lim_{N \rightarrow \infty} 2^{-N} \text{Tr} e^{-itH} \sigma_0^z e^{itH} \sigma_0^z \quad (1.2)$$

other than the old result [1] that at $\Delta = 0$

$$S(t; 0) = [J_0(2t)]^2 \quad (1.3)$$

where $J_0(2t)$ is the Bessel function of order zero.

On the other hand this infinite temperature correlation function is of great interest because of its relation to the theory of spin diffusion [2]- [4] which says that in the limit $t \rightarrow \infty$ if spin diffusion is present in the system then the asymptotic behavior of $S(t, \Delta)$ should be

$$S(t; \Delta) \sim At^{-1/2}. \quad (1.4)$$

In the absence of exact results this asymptotic behavior has been studied by numerical methods for well over 20 years [5]-[9]. By far the most accurate of these numerical studies is the recent work of Fabricius, Löw, and Stolze [9] who have published a beautiful high precision study of the time dependent two spin correlation functions at various temperatures

of the spin 1/2 XXZ antiferromagnet obtained by extrapolating to the thermodynamic limit a finite size exact diagonalization study of systems of size up to $N=16$. From this study the authors were able to give precise estimates of $S(t; \Delta)$ for $\Delta = 1, \cos(.3\pi)$ for the time interval $0 \leq t \leq 4.95$ and they concluded that no evidence of the asymptotic behavior (1.4) could be seen. This supports the conjecture made by the present author [10] and by others [11] that the integrability of the XXZ chain forbids the spin diffusion asymptotic behavior (1.4) and agrees with the absence of diffusion at low temperature found by Narozhny [12] for $-1 \leq \Delta \leq 1$.

However, in [9] there is no positive statement given as to what the true asymptotic behavior of their data might be. Here we show that the numerical results of [9] can be beautifully fit with the form

$$f(t; d, A, B, \gamma, \Omega, t_0) = t^{-d}[A + Be^{-\gamma(t-t_0)} \cos \Omega(t - t_0)] \quad (1.5)$$

which was first suggested in [6] with $d = 1/2$.

To test the validity of the form (1.5) we have computed

$$g(t; d, A) = t^d S(t; \Delta) - A, \quad (1.6)$$

where $S(t; \Delta)$ is given by the numerical values of [9] which were generously sent to us in electronic form, and compared the result with

$$h(t; B, \gamma, \Omega, t_0) = Be^{-\gamma(t-t_0)} \cos \Omega(t - t_0). \quad (1.7)$$

The best results of these comparisons are given graphically in Figs.1 and 2 for $\Delta = 1$ and $\cos(.3\pi)$. From these comparisons we conclude that for $2.2 \leq t \leq 4.95$ the equality

$$S(t; \Delta) = f(t; d, A, B, \gamma, \Omega, t_0) \quad (1.8)$$

holds to a very high degree of precision where

1) for $\Delta = 1$

$$d = .698, \quad A = .245, \quad B = .0581, \quad \gamma = .70, \quad \Omega = 4.36, \quad t_0 = 1.90 \quad (1.9)$$

2) for $\Delta = \cos(.3\pi) = .587 \dots$

$$d = .838, \quad A = .21, \quad B = .114, \quad \gamma = .354, \quad \Omega = 4.06, \quad t_0 = 1.96 \quad (1.10)$$

These results are to be compared with the exact asymptotics of $\Delta = 0$ obtained from (1.3) as

$$S(t; 0) \sim \frac{1}{\pi t} \cos^2(2t - \frac{\pi}{4}) = \frac{1}{2\pi t} \left[1 + \cos(4t - \frac{\pi}{2}) \right] \quad (1.11)$$

which is of the form (1.5) with

$$3) \Delta = 0$$

$$d = 1, \quad A = B = \frac{1}{2\pi} = .159 \dots, \quad \gamma = 0, \quad \Omega = 4, \quad t_0 = \frac{5\pi}{8} = 1.963 \dots \quad (1.12)$$

which is plotted in Fig. 3.

In an attempt to provide some estimate of error in the fitting parameters we plot in Fig. 4 a fit of the case $\Delta = \cos(.3\pi)$ obtained with

$$d = .784, \quad A = .196, \quad B = .104, \quad \gamma = .342, \quad \Omega = 4.06, \quad t_0 = 1.96. \quad (1.13)$$

From comparing the fits of Fig. 2 and 4 we conclude that the estimates of Ω and t_0 are very stable while the exponent d varied by .045. However because the fit which better fits the points with larger t gives the larger value of t we feel that the conclusion that for $t \rightarrow \infty$ the exponent d for $\Delta = \cos(.3\pi)$ is definitely greater the value it has for $\Delta = 1$ is certainly justified.

2. Discussion

The exponent d in (1.9)-(1.12) is always substantially greater than $1/2$. Thus, if $f(t; d, A, B, \gamma, \Omega, t_0)$ of (1.5) does indeed represent the true asymptotic behavior of $S(t; \Delta)$ then the spin diffusion form (1.4) is definitely eliminated. This is in agreement with [9] and is the basis for the claim in the title of this paper. However, it must always be kept in mind that no study for a finite time interval can definitively claim to have seen the true $t \rightarrow \infty$ behavior of a function. This obvious general statement is of particular importance here because numerical studies on the (nonintegrable) classical ($S = \infty$) Heisenberg magnet [13]-[16] show that while a form like (1.5) held for times up to the order of 50 with an exponent d definitely greater than $1/2$ that when times up to 100 were considered the exponent d eventually became the spin diffusion value $d = 1/2$. The belief embodied in the conjecture of the absence of spin diffusion for an integrable model is that there will never be a scale at which the spin diffusion form (1.4) sets in. We further

conjecture for the (nonintegrable) XXZ chains of arbitrary spin $S \geq 1$ that for suitable small times the form (1.5) will be an excellent approximation to the autocorrelation function but that there will exist some time scale such that for times larger than this scale spin diffusion will set in. This scale should increase as the spin S decreases and become infinite for the integrable case of $S = 1/2$. A similar remark holds for the addition of further nearest neighbor interactions to the XXZ chain which also destroy the integrability.

We conclude by remarking that since the data of [9] for $T = \infty$ is so very well fit by (1.5) a similar simple fitting function must exist for finite T . In addition further numerical study should be able to determine the parameters in (1.5) as functions of Δ in the entire range $0 \leq \Delta \leq \infty$. As a guide to such a study we suggest that the parameter $d(\Delta)$ of (1.5) is a monotonic nonincreasing function of Δ and that $\lim_{\Delta \rightarrow \infty} d(\Delta) = 1/2$.

Acknowledgments

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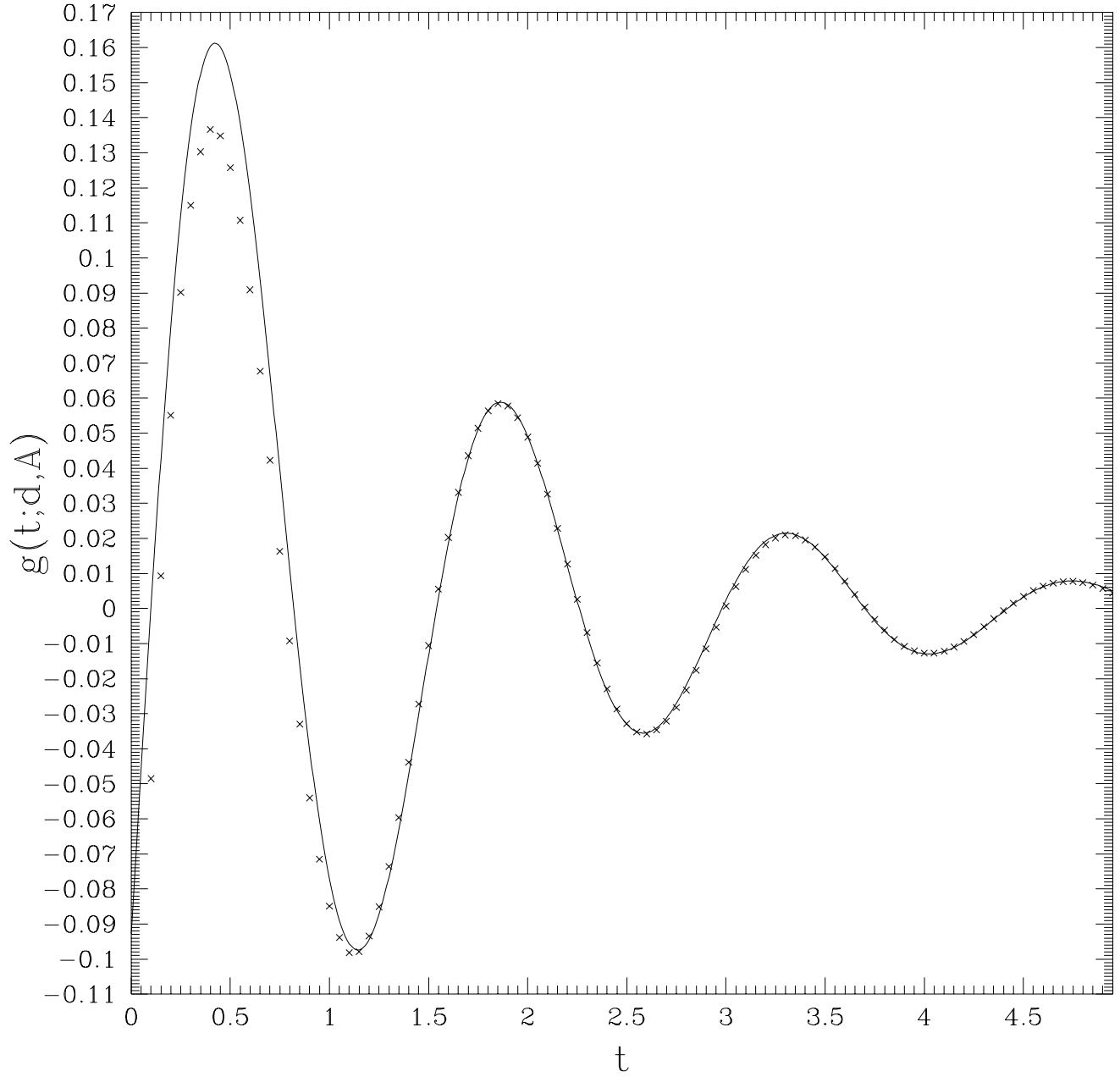


Fig. 1 Comparison of the numerical data of [9] for $\Delta = 1$ with the form (1.5) with $d = .698$, $A = .245$, $B = .0581$, $\gamma = .7$, $\Omega = 4.36\dots$, $t_0 = 1.90$. The points are the function $g(t; , d, A)$ (1.6) obtained from the data of [9]. The continuous curve is $h(t; B, \gamma, \Omega, t_0)$ of (1.7) with $B = .0581$, $\gamma = .70$, $\Omega = 4.36$, $t_0 = 1.90$.

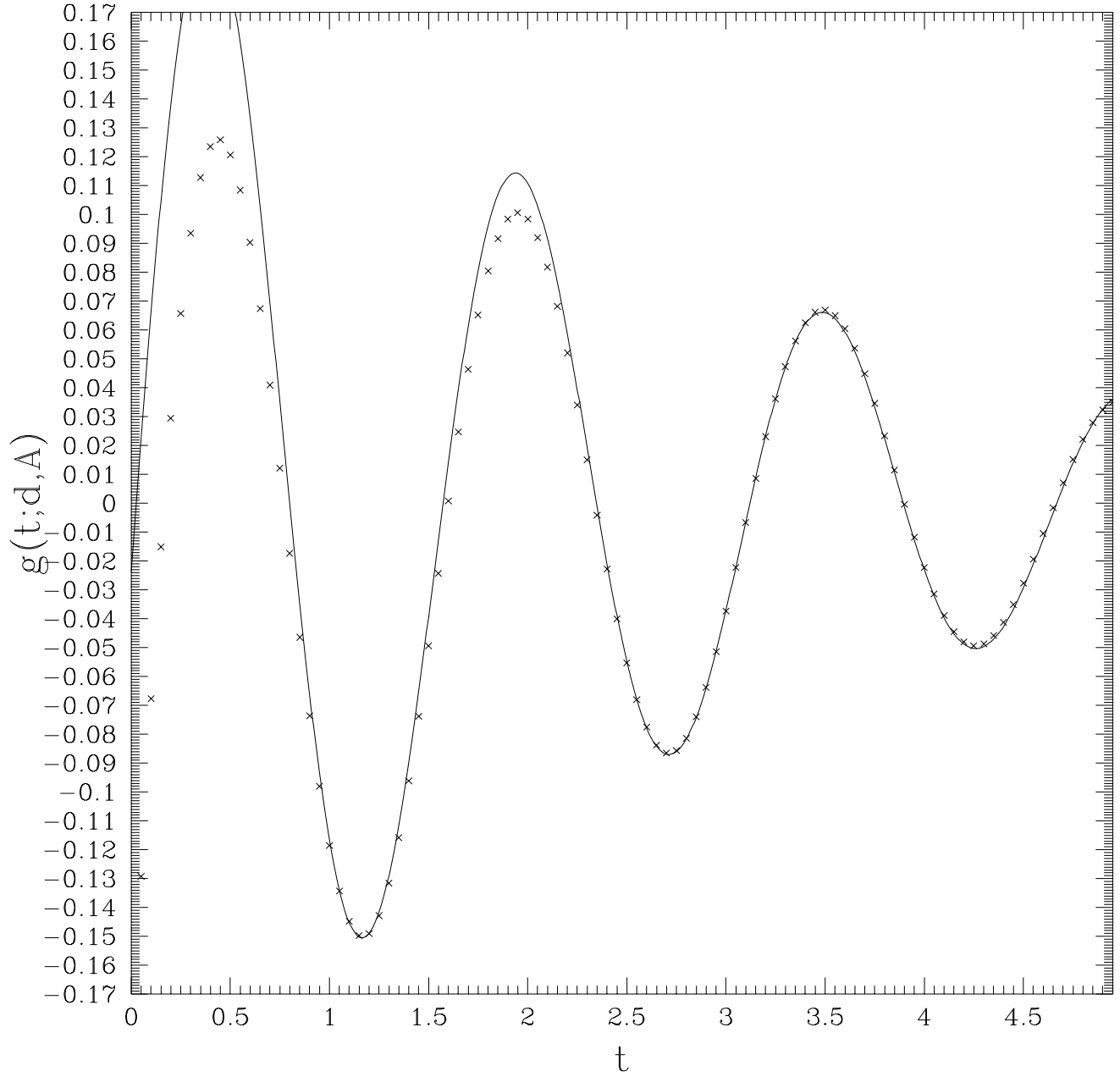


Fig. 2 Comparison of the numerical data of [9] for $\Delta = \cos(.3\pi)$ with the form (1.5) with $d = .838$, $A = .210$, $B = .114$, $\gamma = .354$, $\Omega = 4.06$, $t_0 = 1.96$. The points are the function $g(t; , d, A)$ (1.6) obtained from the data of [9]. The continuous curve is $h(t; B, \gamma, \Omega, t_0)$ of (1.7) with $B = .114$, $\gamma = .354$, $\Omega = 4.06$, $t_0 = 1.96$.

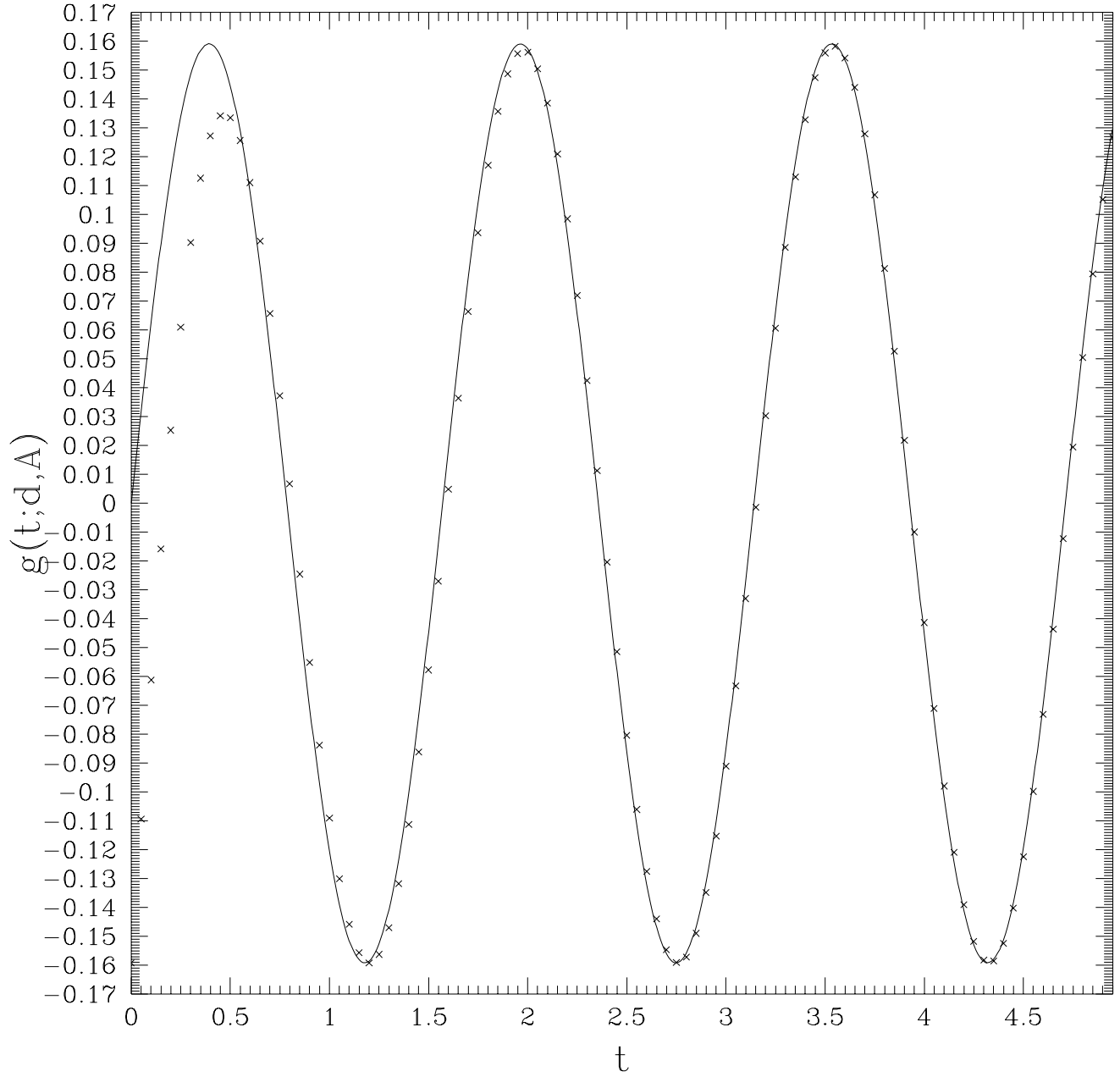


Fig. 3 Comparison of the exact result (1.3) for $\Delta = 0$ with the form (1.5) with $d = 1.0$, $A = B = \frac{1}{2\pi} = .159\dots$, $\gamma = 0$, $\Omega = 4.0$, $t_0 = \frac{5\pi}{8} = 1.963\dots$. The points are the function $g(t; , d, A)$ (1.6) obtained from (1.3). The continuous curve is $h(t; B, \gamma, \Omega, t_0)$ of (1.7) with $B = \frac{1}{2\pi} = .159\dots$, $\gamma = 0.0$, $\Omega = 4.0$, $t_0 = \frac{5\pi}{8} = 1.963\dots$.

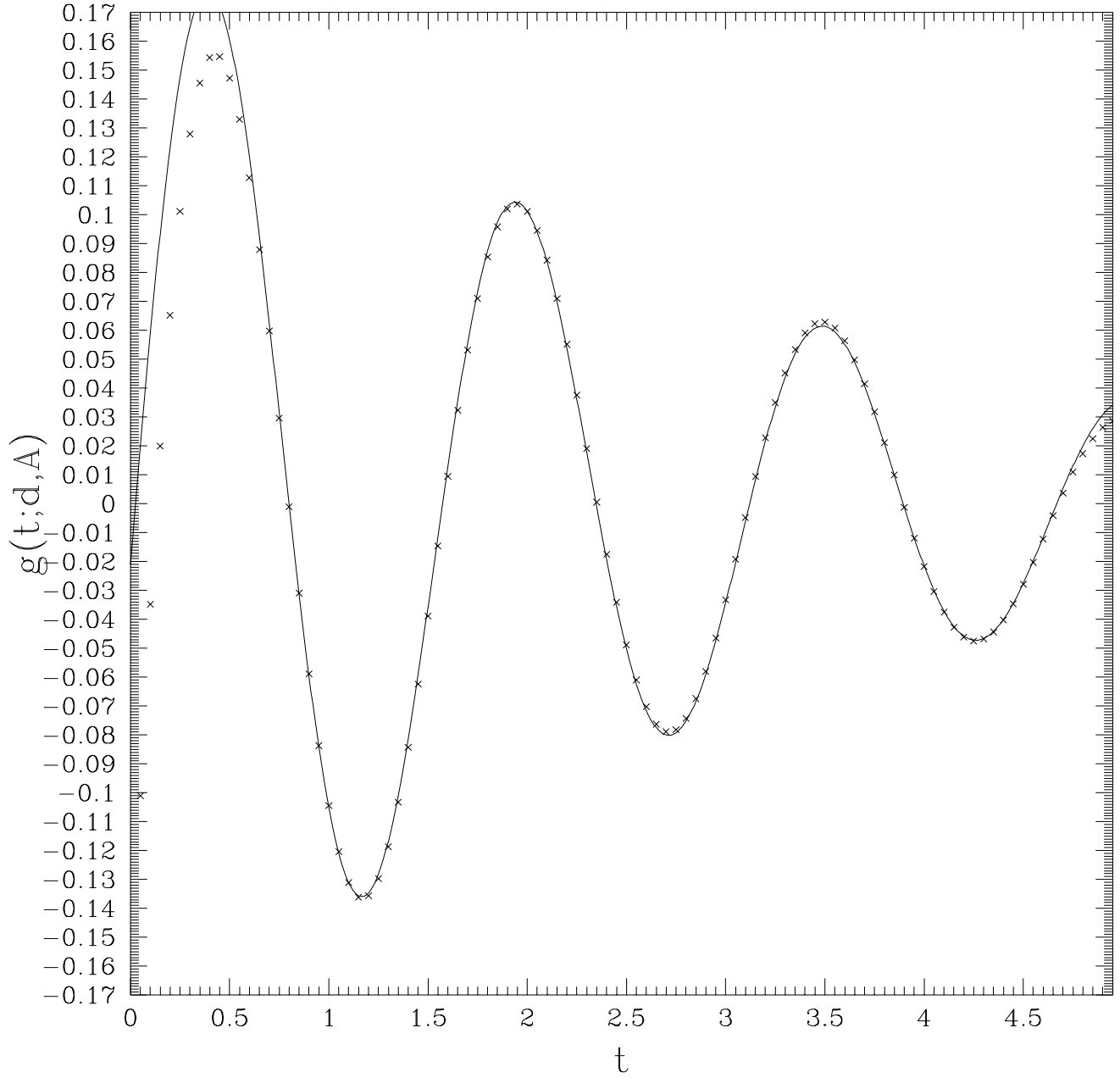


Fig. 4 Comparison of the numerical data of [9] for $\Delta = \cos(.3\pi)$ with the form (1.5) with $d = .784$, $A = .196$, $B = .104$, $\gamma = .342$, $\Omega = 4.06$, $t_0 = 1.96$. The points are the function $g(t; , d, A)$ (1.6) obtained from the data of [9]. The continuous curve is $h(t; B, \gamma, \Omega, t_0)$ of (1.7) with $B = .104$, $\gamma = .342$, $\Omega = 4.06$, $t_0 = 1.96$.

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